Energetic coupling between Phase Field Crystal and Field Dislocation Mechanics

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Résumé pour : Poster

Over diffusive time scales, dislocation mechanics has been modeled using the Phase Field Crystal (PFC) and Field Dislocation Mechanics (FDM) approaches. The PFC model describes a time-averaged atomic density of a crystal at microscopic lengths and provides a lattice-level crystallographic "landscape" that naturally encodes defect topology, but its evolution is diffusive and misrepresents fast elastic relaxation. FDM is the state-of-the-art theory for modeling dislocation mechanics, but it fails to naturally maintain compact dislocation cores while transporting them with stress-dependent velocities when no non-convex energetic terms carrying crystallographic information are provided. PFC and FDM are, therefore, seemingly complementary to each other, and coupling them could potentially yield a framework that allows continuum mechanics-based modeling of compact dislocation cores being transported under stress-dependent velocities. To that end, an energetic coupling using an L^2 penalty on the difference between the elastic distortion from FDM and configurational distortion from PFC was proposed by Acharya and Viñals [1]. In this work, we theoretically and numerically analyze the advantages and limitations of this coupling.

[1] A. Acharya, J. Viñals. "Field dislocation mechanics and phase field crystal models," in *Phys. Rev. B*, vol. 102, pp. 064109, 2020.